Benjamin F. Gherman
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CURRENT EMPLOYMENT

• **California State University, Sacramento.** Sacramento, California, 2006-present.
  · **Professor**, September 2018-present.
  · **Associate Professor**, September 2012-August 2018.
  · **Assistant Professor**, September 2006-August 2012.
    Classes Taught: Chemical Calculations, General Chemistry I, Physical Chemistry Lecture I and II, Introduction to Physical Chemistry, Computational Chemistry.
    Research Focus: Computational bioinorganic, organometallic, and organic chemistry.

EDUCATION

• **University of Minnesota (Twin Cities)**, Minneapolis, Minnesota, 2003-2006.
  · **Post-doctoral associate**, September 2003-July 2006.
    Project Title: Modeling Oxygen Activation by Monocopper Enzyme Sites
• **Columbia University**, New York, New York, 1998-2003.
  · **Ph. D.** Chemistry, October 2003.
    Dissertation Title: Using Quantum Chemical and Mixed Quantum Chemical/ Molecular Mechanics Methods to Study Reaction Mechanisms in Enzymes
    Advisor: Richard A. Friesner
  · **M. Phil.** Chemistry, February 2002.
  · **M. A.** Chemistry, October 1999.
• **Carnegie Mellon University**, Pittsburgh, Pennsylvania, 1994-1998.
  · **B. S.** Chemistry (with Computational Chemistry option), May 1998.
  · **B. S.** Mathematics, May 1998.

PROFESSIONAL EXPERIENCE

Research Experience

Current Research, *Department of Chemistry, California State University, Sacramento*
  · September 2006 – present.
  - Modeling the catalytic chemistry in the enzyme peptide deformylase (PDF) and in non-heme iron halogenases. The former is an essential component in the life cycle of bacteria and an ideal new target for antibacterial therapies; the latter catalyzes chemoselective halogenation of natural products. For each enzyme, the role of the metal ion and the effect of ligand modifications on the catalytic reaction are being investigated. New biomimetic model systems for the enzyme active sites are being designed to better replicate the enzymatic catalysis.
  - Determining the reactivity of enediynes and related compounds with respect to their tendency to cyclize upon thermal or photo-activation (project in collaboration with Prof. John Spence, CSU, Sacramento Chemistry Dept.). The compounds can be used as pro-drugs for DNA cleavage and have application in chemotherapy. Thermodynamics and kinetics of the cyclization reactions along multiple pathways are calculated; at the same time, UV/Vis spectra for the compounds are calculated and the associated electronic excitations are characterized.
  - Investigation of the electrochemistry of metal-salen compounds and their potential for use in the synthesis of pharmaceutically relevant organic compounds (project in collaboration with Prof. James Miranda, CSU, Sacramento Chemistry Dept.). One aspect of research involves the development of a computational chemistry method for the accurate determination of reduction potentials for metal-salens. A second research direction involves the study of the mechanism and kinetics for electroreductive cyclization (ERC) reactions catalyzed by reduced metal-salens.

• **Post-doctoral Research,** *Department of Chemistry, University of Minnesota (Twin Cities).*
  · September 2003 – July 2006. Professor Christopher J. Cramer and Professor William B. Tolman, advisors.
      ♦ Studied the catalytic mechanisms of the dopamine ß-monooxygenase (DßM) and peptidylglycine α-hydroxylating monooxygenase (PHM) enzymes by quantum chemical modeling of the active sites. The effects of different coordination environments for the copper atoms on dioxygen activation and substrate hydroxylation are determined. This work represents the first application of theoretical methods to model specific reaction mechanisms in these enzymes and will greatly increase understanding of the reaction chemistry of monocopper complexes in general.
      ♦ Modeled dioxygen activation and substrate hydroxylation in biomimetic monocopper complexes being developed in the Tolman group. This work was carried out in conjunction with parallel experimental studies in the Tolman group.
      ♦ Mentored and collaborated with an undergraduate student as a part of these two projects, leading to publication (see #3 in publications).
• **Graduate Research,** *Department of Chemistry, Columbia University.*
  · January 1999 – August 2003. Professor Richard A. Friesner, advisor.
      ♦ Based upon *ab initio* quantum chemical studies on a large-scale model, proposed for the first time complete and realistic catalytic cycles for dioxygen activation and methane hydroxylation by soluble methane monooxygenase, a metalloenzyme that is found in methanotrophic bacteria. Computational results were found to be fully consistent with and provide explanation for experimental data. Further work on this system succeeded in explaining the different rates and kinetic isotopic effects seen in the reaction of methane monooxygenase with substituted methane substrates.
      ♦ Use of a novel mixed quantum mechanics/molecular mechanics method (QM/MM) to determine the origin of the different rates for the deacylation step in the hydrolysis of ß-lactam antibiotics performed by penicillin-binding proteins and class-C ß-lactamases. This research played a role in understanding the differences in reactivity of the two enzymes towards ß-lactam antibiotics and contributed to an understanding of the mechanism of bacterial antibiotic resistance.
• **Undergraduate Research,** Department of Chemistry, Carnegie Mellon University.
  · May 1995 - August 1995, May 1996 - August 1996, May 1997 - August 1997, January 1998 - May 1998. Professor David Yaron, advisor.
      ♦ Studied the electronics of conjugated polymers (in particular, polyacetylene) using semi-empirical quantum methods and developed C++ computer code to implement the semi-empirical INDO quantum chemical method.

Teaching Experience

• **Course Assistant,** *Department of Chemistry, Columbia University.*
  · General Chemistry I and II, January 2000 - May 2001. Aided in various aspects of the courses, including:
      ♦ maintaining the course web page
      ♦ assisting in exam preparations and administrations
      ♦ advising teaching assistants
      ♦ answering questions on the class electronic bulletin board
• **Teaching Assistant,** *Department of Chemistry, Columbia University.*
  · August 1998 - December 1999. Taught general chemistry I and II recitations.
• **Teaching Assistant,** *Department of Mathematics, Carnegie Mellon University.*
  · August 1996 - May 1997. Taught calculus I and II recitations.

Teaching Development

• **Center for Teaching and Learning, California State University, Sacramento**.
  · *Teach ON!-line Summer Camp!*, June 2020 - July 2020.
    ♦ Included topics such as converting existing classes into effective online courses, improving the virtual experience for students, and maximizing learning, engagement, and success.
• **Center for Teaching and Learning Services, University of Minnesota (Twin Cities)**.
  · *Preparing Future Faculty Program*, letter of recognition and certificate of program participation, December 2005.
  · *"Practicum for Future Faculty" graduate course in the Preparing Future Faculty Program,* September 2005 – December 2005.
    ♦ Designed to give opportunities to apply pedagogical theories and methods and to enhance understandings of the faculty role in higher education. Includes a mentoring opportunity in which participants teach three class sessions and explore the faculty role with the guidance of a faculty mentor (at Augsburg College, Minneapolis, MN under Prof. Arlin Gyberg, Chemistry Dept.).
  · *"Using Electronic Discussions" workshop,* April 2005.
    ♦ Included topics such as asynchronous (threaded) online discussions and the ways they may be used in face-to-face classes.
  · *"PowerPoint Reconsidered" workshop,* March 2005.
    ♦ Included topics such as common problems when teaching with PowerPoint and pedagogically sound ways use to this presentation technology.
  · *"Teaching in Higher Education" graduate course in the Preparing Future Faculty Program,* September 2004 – December 2004.
    ♦ Included topics such as active learning strategies, educational theory and practice, diversity of learners, and course and curriculum design. Designed with overall goal of training responsive and reflective teachers.
  · *Preparing Future Faculty Retreat*, May 2004
    ♦ Included workshops on "E-tivities: Engaging Students with Technology" and "Presenting Content: Lively & Practical Approaches"
• **Graduate School of Arts and Sciences, Columbia University**.
  · *Teaching Program Workshop*, October 2001. "Teaching: Course Web Pages and Courseworks"

AWARDS
• California State University, Sacramento Faculty Research Incentive Grant, 2019.
• California State University, Sacramento research and creativity award, 2018.
• California State University, Sacramento Provost's Research Incentive Fund grant, 2014.
• California State University, Sacramento University Enterprises, Inc. Faculty Grant, 2014.
• California State University, Sacramento College of Natural Sciences and Mathematics faculty promotion development grant, 2012.
• California State University, Sacramento College of Natural Sciences and Mathematics faculty promotion development grant, 2011.
• California State University, Sacramento research and creativity award, 2011.
• California State University, Sacramento pedagogy enhancement award, 2011.
• California State University CSUPERB faculty-student collaborative research seed grant, 2010.
• California State University, Sacramento pedagogy enhancement award, 2010.
• California State University, Sacramento College of Natural Sciences and Mathematics faculty promotion development grant, 2010 (twice).
• California State University, Sacramento College of Natural Sciences and Mathematics faculty travel grant, 2009.
• California State University, Sacramento research and creativity award, 2009.
• California State University, Sacramento pedagogy enhancement award, 2009.
• California State University, Sacramento probationary faculty development grant, 2008.
• California State University, Sacramento College of Natural Sciences and Mathematics, summer project grant, 2008.
• California State University, Sacramento research and creativity award, 2008.
• California State University, Sacramento pedagogy enhancement award, 2008.
• Wiley-International Journal of Quantum Chemistry Young Investigator Award, 2008.

- California State University, Sacramento University Enterprises, Inc., faculty professional development award, 2008.
- California State University CSUPERB faculty travel grant (twice), 2008.
- Developmental project allocation (title: "Using Mixed Quantum Mechanics/Molecular Mechanics Calculations to Assess the Effects of Mutations on the Catalytic Activity of Peptide Deformylase") of 24,000 service units from the National Center for Supercomputing Applications (NCSA), 2007-2008.
- NIH National Research Service Award Post-doctoral Fellowship, titled "Modeling Oxygen Activation by Monocopper Enzyme Sites," 2003-2006.
- NIH Biophysics Training Grant, Columbia University, 2001-2003.
- Jack Miller Award for graduate teaching, Columbia University, 2000.
- U.S. Department of Defense National Defense Science and Engineering Graduate Fellowship, Columbia University, 1998-2001.
- Member Phi Beta Kappa Honor Society, Carnegie Mellon University, 1998.
- College awardee of the Society of Analytical Chemists of Pittsburgh, Carnegie Mellon University, 1998.
- Lubrizol scholarship for chemistry majors, Carnegie Mellon University, 1997.
- Warner Prize for sophomore chemistry majors, Carnegie Mellon University, 1996.
- Member Phi Kappa Phi Honor Society, Carnegie Mellon University, 1996.
- Member Lambda-Sigma National Sophomore Honor Society, Carnegie Mellon University, 1995 and Hall of Fame member, 1996.
- University scholarship, Carnegie Mellon University, 1995-1998.
- Dean's high honor list, Carnegie Mellon University, all four academic years 1994-1998.

PUBLICATIONS

(undergraduate students denoted with asterisk; graduate students denoted with two asterisks)

1. S. A. Valenzuela*, A. J. Cortés*, Z. J. E. Tippins*, M. H. Daly*, T. E. Keel*, B. F. Gherman, J. D. Spence. "Effect of Extended Benzannelation Orientation on Bergman and Related Cyclizations of Isomeric Quinoxalenediynes." *J. Org. Chem.*, **82**, 13297-13312 (2017).

2. J. S. Fell**, D. M. Steele*, T. C. Hatcher III*, B. F. Gherman. "Electronic Effects on the Reaction Mechanism of the Metalloenzyme Peptide Deformylase." *Theor. Chem. Acc.*, **134**, 71 (2015).

3. J. M. Yates**, J. S. Fell**, J. A. Miranda, B. F. Gherman. "Metal-Salens as Catalysts in Electroreductive Cyclization and Electrohydrocyclization: Computational and Experimental Studies." *J. Electrochem. Soc.*, **160**, G3080-G3090 (2013).

4. J. M. Yates**, J. S. Fell**, J. A. Miranda, B. F. Gherman. "Metal-Salens as Catalysts in Electroreductive Cyclization and Electrohydrocyclization: Computational and Experimental Studies." *ECS Trans.*, **50**, 5-15 (2013).

5. J. D. Spence, A. C. Rios*, M. A. Frost*, C. M. McCutcheon*, C. D. Cox*, S. Chavez*, R. Fernandez*, B. F. Gherman. "Syntheses, Thermal Reactivities, and Computational Studies of Aryl-Fused Quinoxalenediynes: Effect of Extended Benzannelation on Bergman Cyclization Energetics." *J. Org. Chem.*, **77**, 10329-10339 (2012).

6. N. G. Spiropulos, E. A. Standley, I. R. Shaw, B. L. Ingalls, B. Diebels, S. V. Krawczyk*, B. F. Gherman, A. M. Arif, E. C. Brown. "Synthesis of Zinc and Cadmium *O*-Alkyl Thiocarbonate and Dithiocarbonate Complexes and a Cationic Zinc Hydrosulfide Complex." *Inorg. Chim. Acta*, **386**, 83-92 (2012).

7. N. V. Korovina*, M. L. Chang*, T. T. Nguyen*, H. J. Walker, R. P. Fernandez*, M. M. Olmstead, B. F. Gherman, J. D. Spence. "Syntheses and Reactivity of Naphthalenyl-Substituted Arenediynes." *Org. Lett.*, **13**, 3660-3663 (2011).

8. M. F. Brown*, B. F. Gherman. "Importance of Iron as the Metal Ion in Peptide Deformylase: A Biomimetic Computational Study." *Theor. Chem. Acc.*, **128**, 137-146 (2011).

9. S. B. Bateni*, K. R. England*, A. T. Galatti*, H. Kaur*, V. A. Mendiola*, A. R. Mitchell*, M. H. Vu*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Calculated Electron Affinities for Metal-Salen Compounds." *Beilstein J. Org. Chem.*, **5** (2009), doi:10.3762/bjoc.5.82.

10. B. F. Gherman and C. J. Cramer. "Quantum Chemical Studies of Molecules Incorporating a $Cu_2O_2^{2+}$ Core." *Coord. Chem. Rev.*, **253**, 723-753 (2009).

11. A. H. Winter, D. E. Falvey, C. J. Cramer, B. F. Gherman. "Benzylic Cations with Triplet Ground States: Computational Studies of Aryl Carbenium Ions, Silylenium Ions, Nitrenium Ions and Oxenium Ions Substituted with *meta* Pi Donors." *J. Am. Chem. Soc.*, **129**, 10113-10119 (2007).

12. N. E. Schultz, B. F. Gherman, C. J. Cramer, D. G. Truhlar. "Pd$_n$CO (n = 1,2): Accurate ab Initio Bond Energies, Geometries, and Dipole Moments and the Applicability of Density Functional Theory for Fuel Cell Modeling." *J. Phys. Chem. B*, **110**, 24030-24046 (2006).

13. L. R. M. Hill, B. F. Gherman, N. W. Aboelella, C. J. Cramer, W. B. Tolman. "Electronic Tuning of β-Diketiminate Ligands with Fluorinated Substituents: Effects on the O_2-Reactivity of Mononuclear Cu(I) Complexes." *Dalton Trans.* 4944-4953 (2006).

14. D. E. Heppner, B. F. Gherman, W. B. Tolman, C. J. Cramer. "Can an Ancillary Ligand Lead to a Thermodynamically Stable End-on 1:1 Cu-O_2 Adduct Supported by a β-Diketiminate Ligand?" *Dalton Trans.* 4773-4782 (2006).

15. B. F. Gherman, W. B. Tolman, C. J. Cramer. "Characterization of the Structure and Reactivity of Monocopper-Oxygen Complexes Supported by β-Diketiminate and Anilido-Imine Ligands." *J. Comput. Chem.* **27**, 1950-1961 (2006).

16. N. W. Aboelella, B. F. Gherman, L. M. Hill, J. T. York, N. Holm, V. G. Young, Jr., C. J. Cramer, W. B. Tolman. "Effects of Thioether Substituents on the O_2 Reactivity of β-Diketiminate-Cu(I) Complexes: Probing the Role of the Methionine Ligand in Copper Monooxygenases." *J. Am. Chem. Soc.* **128**, 3345-3358 (2006).

17. B. F. Gherman, D. E. Heppner, W. B. Tolman, C. J. Cramer. "Models for Dioxygen Activation by the Cu_B Site of DβM and PHM." *J. Biol. Inorg. Chem.* **11**, 197-205 (2006).

18. C. R. Kinsinger, B. F. Gherman, L. Gagliardi, C. J. Cramer. "How Useful Are Vibrational Frequencies of Isotopomeric O_2 Fragments for Assessing Local Symmetry? Some Simple Systems and the Vexing Case of a Galactose Oxidase Model." *J. Biol. Inorg. Chem.* **10**, 778-789 (2005).

19. A. M. Reynolds, B. F. Gherman, C. J. Cramer, W. B. Tolman. "Characterization of a 1:1 Cu/O_2 Adduct Supported by an Anilido-Imine Ligand." *Inorg. Chem.* **44**, 6989-6997 (2005).

20. N.W. Aboelella, W. W. Brennessel, V. G. Young, Jr., S. Kryatov, E. Rybak-Akimova, R. Sarangi, E. I. Solomon, B. F. Gherman, C. J. Cramer, and W. B. Tolman. "Dioxygen Activation at a Single Copper Site: Structure, Bonding, and Mechanism of Formation of 1:1 Cu/O_2 Adducts." *J. Am. Chem. Soc.* **126**, 16896-16911 (2004).

21. B. F. Gherman and C. J. Cramer. "Modeling the Peroxide/Superoxide Continuum in 1:1 Side-on Adducts of O_2 with Cu." *Inorg. Chem.* **43**, 7281-7283 (2004).

22. B. F. Gherman, S. J. Lippard, and R. A. Friesner. "Substrate hydroxylation in methane monooxygenase: quantitative modeling via mixed quantum mechanics/molecular mechanics techniques." *J. Am. Chem. Soc.* **127**, 1025-1037 (2005).

23. B. F. Gherman, S. Goldberg, V. W. Cornish, and R. A. Friesner. "Mixed Quantum Mechanical/Molecular Mechanical (QM/MM) Study of the Deacylation Reaction in a Penicillin Binding Protein (PBP) Versus in a Class C β-Lactamase."*J. Am. Chem. Soc.* **126**, 7652-7664 (2004).

24. B. F. Gherman, S. J. Lippard, and R. A. Friesner. "Dioxygen activation in methane monooxygenase: a theoretical study." *J. Am. Chem. Soc.* **126**, 2978-2990 (2004).

25. R. A. Friesner, M.-H. Baik, V. Guallar, B. F. Gherman, M. Wirstam, R. B. Murphy, and S. J. Lippard. "How iron-containing proteins control dioxygen chemistry: a detailed atomic level description via accurate quantum chemical and mixed quantum mechanics/molecular mechanics calculations." *Coord. Chem. Rev.* **238-239**, 267-290 (2003).

26. M.-H. Baik, B. F. Gherman, R. A. Friesner, and S. J. Lippard. "Hydroxylation of methane by non-heme diiron enzymes. A molecular orbital analysis of C–H bond activation by reactive intermediate Q." *J. Am. Chem. Soc.* **124**, 14608-14615 (2002).

27. V. Guallar, B. F. Gherman, S. J. Lippard, and R. A. Friesner. "Quantum chemical studies of methane monooxygenase: comparison with P450." *Curr. Opin. Chem. Biol.* **6**, 236-242 (2002).

28. V. Guallar, B. F. Gherman, W. H. Miller, S. J. Lippard, and R. A. Friesner. "Dynamics of alkane hydroxylation at the non-heme diiron center in methane monooxygenase." *J. Am. Chem. Soc.* **124**, 3377-3384 (2002).

29. B. F. Gherman, B. D. Dunietz, D. A. Whittington, S.J. Lippard, and R. A. Friesner. "Activation of the C-H bond of methane by intermediate Q of methane monooxygenase: a theoretical study." *J. Am. Chem. Soc.* **123**, 3836-3837 (2001).

30. B. F. Gherman, R. A. Friesner, T.-H. Wong, Z. Min, and R. Bersohn. "Photodissociation of acetaldehyde: the CH_4 + CO channel." *J. Chem. Phys.* **114**, 6128-6133 (2001).

31. I. Ivanov, B. F. Gherman, and D. Yaron. "Comparison of the INDO band structures of polyacetylene, polythiophene, polyfuran, and polypyrrole." *Synthetic Metals* **116**, 111-114 (2001).

32. E. Moore, B. F. Gherman, and D. Yaron. "Coulomb screening and exciton binding energies in conjugated polymers." *J. Chem. Phys.* **106**, 4216-4227 (1997).

33. D. Yaron, E. Moore, and B. F. Gherman. "Models of electron-hole screening and exciton binding in conjugated polymers." *Materials Research Society Symposium Proceedings* **413**, 541-546 (1996).

PRESENTATIONS
(presenter underlined; undergraduate students denoted with asterisk; graduate students denoted with two asterisks)
1. A. Waltonen**, M. McAnally*, B. F. Gherman. "Biomimetic Modeling of Non-Heme Iron Halogenase Enzymes." 2024 West Coast Theoretical Chemistry, University of California, Merced; Merced, California; May 2024.
2. L. Ly*, B. F. Gherman, J. D. Spence. "Radical anion cyclization of substituted quinoxalenediynes." (poster) 2023 Annual Undergraduate American Chemical Society Research Conference for Northern California; Moraga, California; May 2023.
3. G. Barakat*, K. D. Daniels*, B. F. Gherman, J. A. Miranda. "Correlation between substituent Hammett σ_p parameters and UV-vis absorptions for substituted metal-salens." (poster) 2023 Annual Undergraduate American Chemical Society Research Conference for Northern California; Moraga, California; May 2023.
4. M. Cihak**, B. F. Gherman, J. A. Miranda. "Ni-Salen and Zn-Salen Catalyzed Electroreductive Cyclization Reactions: An in Depth Look at Mechanisms and Stereoselectivity." 35th California State University Biotechnology Symposium; Santa Clara, California; January 2023.
5. A. Waltonen**, M. McAnally*, B. F. Gherman. "Biomimetic Modeling of Non-Heme Iron Halogenase Enzymes." 35th California State University Biotechnology Symposium; Santa Clara, California; January 2023.
6. M. Cihak**, B. F. Gherman, J. A. Miranda. "Ni-Salen and Zn-Salen Catalyzed Electroreductive Cyclization Reactions: An in Depth Look at Mechanisms and Stereoselectivity." 2022 Inorganic Chemistry Symposium, University of California, Davis; Davis, California, November 2022.
7. A. Waltonen**, M. McAnally*, B. F. Gherman. "Biomimetic Modeling of Non-Heme Iron Halogenase Enzymes." 2022 Inorganic Chemistry Symposium, University of California, Davis; Davis, California, November 2022.
8. B. F. Gherman. "Using Computational Chemistry and Biomimetic Models to Investigate Catalysis at Enzyme Active Sites." California State University, Chico; Chico, CA; April 2022.
9. B. F. Gherman. "Using computational chemistry and biomimetic models to study enzyme chemistry." Summer Seminar in Chemical Theory and Computation (Northern California CSU); July 2021.
10. M. McAnally*, D. J. Lindsay*, B. F. Gherman. "Biomimetic Modeling of Non-Heme Iron Halogenase Enzymes." (poster) 32nd California State University Biotechnology Symposium; Santa Clara, California; January 2020.
11. D. J. Lindsay*, B. F. Gherman. "Computational Study of the Reactivity and Chemoselectivity of Non-Heme Iron Halogenases." (poster) 31st California State University Biotechnology Symposium; Anaheim, California; January 2019.
12. A. Waltonen*, B. F. Gherman, J. D. Spence. "Biradical Stability in Bergman Cyclization Products from Benzannelated Enediynes." (poster) 31st California State University Biotechnology Symposium; Anaheim, California; January 2019.
13. B. H. Bohne*, T. Keel*, M. H. Daly*, B. F. Gherman, J. D. Spence. "Using Steric Effects to Promote the Cyclization of Angularly Benzannelated Enediynes." (poster) 30th Annual Undergraduate American Chemical Society Research Conference for Northern California; Oakland, California; April 2018.
14. A. Waltonen*, B. F. Gherman, J. D. Spence. "Biradical Stability in Bergman Cyclization Products from Benzannelated Enediynes." (poster) 30th Annual Undergraduate American Chemical Society Research Conference for Northern California; Oakland, California; April 2018.
15. B. H. Bohne*, T. Keel*, M. H. Daly*, B. F. Gherman, J. D. Spence. "Using Steric Effects to Promote the Cyclization of Angularly Benzannelated Enediynes." (poster) 30th California State University Biotechnology Symposium; Santa Clara, California; January 2018.
16. T. Keel*, M. H. Daly*, B. F. Gherman, J. D. Spence. "Using Electronics and Sterics to Affect the Cyclization of Angularly Benzannelated Enediynes." (poster) 29th Annual Undergraduate American Chemical Society Research Conference for Northern California; San Jose, California; May 2017.
17. K. A. Hoang*, D. Powers*, C. Q. Li**, B. F. Gherman, J. D. Spence. "Computational Prediction of Cyclization Pathway Restriction with Enyne-ynones." (poster) 29th Annual Undergraduate American Chemical Society Research Conference for Northern California; San Jose, California; May 2017.
18. T. Keel*, M. H. Daly*, B. F. Gherman, J. D. Spence. "Using Electronics and Sterics to Affect the Cyclization of Angularly Benzannelated Enediynes." (poster) 253rd American Chemical Society National Meeting; San Francisco, California; April 2017.
19. K. A. Hoang*, C. Q. Li**, B. F. Gherman, J. D. Spence. "Steric Effects in the Computational Modeling of Enediynone Cyclization Reactions." (poster) 253rd American Chemical Society National Meeting; San Francisco, California; April 2017.
20. L. V. Bellini**, M. Cihak*, B. E. Silva*, B. F. Gherman, J. A. Miranda. "Mechanism for the Stereoselectivity in Metal-Salen Catalyzed Electroreductive Cyclization Reactions." (poster) 253rd American Chemical Society National Meeting; San Francisco, California; April 2017.

21. K. A. Hoang*, C. Q. Li**, <u>B. F. Gherman</u>, J. D. Spence. "Steric Effects in the Computational Modeling of Cyclization Reactions of Enyne-Enones." 253rd American Chemical Society National Meeting; San Francisco, California; April 2017.

22. <u>K. A. Hoang*</u>, C. Q. Li**, B. F. Gherman, J. D. Spence. "Steric Effects in the Computational Modeling of Cyclization Reactions of Enediynones." (poster) 29th California State University Biotechnology Symposium; Santa Clara, California; January 2017.

23. <u>L. Bellini**</u>, M. Cihak*, B. E. Silva*, B. F. Gherman, J. A. Miranda. "Mechanism for the Stereoselectivity in Metal-Salen Catalyzed Electroreductive Cyclization Reactions." (poster) 29th California State University Biotechnology Symposium; Santa Clara, California; January 2017.

24. <u>K. A. Hoang*</u>, C. Q. Li**, B. F. Gherman, J. D. Spence. "Steric Effects in the Computational Modeling of Cyclization Reactions of Enediynones." (poster) 28th Annual Undergraduate American Chemical Society Research Conference for Northern California; Moraga, California; April 2016.

25. <u>M. H. Daly*</u>, B. F. Gherman, J. D. Spence. "Electronic and Steric Effects on the Cyclization of Angularly Benzannelated Enediynes." (poster) 28th Annual Undergraduate American Chemical Society Research Conference for Northern California; Moraga, California; April 2016.

26. <u>K. A. Hoang*</u>, C. Q. Li**, B. F. Gherman, J. D. Spence. "Steric Effects in the Computational Modeling of Cyclization Reactions of Dieneynones." (poster) 28th California State University Biotechnology Symposium; Anaheim, California; January 2016.

27. <u>M. H. Daly*</u>, B. F. Gherman, J. D. Spence. "Electronic and Steric Effects on the Cyclization of Angularly Benzannelated Enediynes." (poster) 28th California State University Biotechnology Symposium; Anaheim, California; January 2016.

28. <u>K. A. Hoang*</u>, C. Q. Li**, B. F. Gherman, J. D. Spence. "Steric Effects in the Computational Modeling of Cyclization Reactions of Dieneynones." (poster) 27th Annual Undergraduate American Chemical Society Research Conference for Northern California; Santa Cruz, California; May 2015.

29. <u>D. Powers*</u>, C. Q. Li**, B. F. Gherman, J. D. Spence. "Computational Study of the Cyclization Product Pathway Restriction of Substituted Enediynones." (poster) 27th Annual Undergraduate American Chemical Society Research Conference for Northern California; Santa Cruz, California; May 2015.

30. <u>M. Cihak*</u>, B. E. Silva*, B. F. Gherman, J. A. Miranda. "Mechanism and Prospect for Stereoselectivity in Metal-Salen Catalyzed Electroreductive Cyclization Reactions." (poster) 27th Annual Undergraduate American Chemical Society Research Conference for Northern California; Santa Cruz, California; May 2015.

31. <u>A. Nguyen*</u>, B. F. Gherman, J. D. Spence. "Assessment of the Contribution of Dispersion Interactions in the Energetics of Bergman Cyclization of Enediynes." (poster) 27th Annual Undergraduate American Chemical Society Research Conference for Northern California; Santa Cruz, California; May 2015.

32. <u>B. F. Gherman</u>. "Effect of the Metal Center and Active Site Ligands on Catalysis in the Metalloenzyme Peptide Deformylase." California State University, Sacramento; Sacramento, California; April 2015.

33. <u>M. Cihak*</u>, B. E. Silva*, B. F. Gherman, J. A. Miranda. "Mechanism and Prospect for Stereoselectivity in Metal-Salen Catalyzed Electroreductive Cyclization Reactions." (poster) 27th California State University Biotechnology Symposium; Santa Clara, California; January 2015.

34. <u>A. Nguyen*</u>, B. F. Gherman, J. D. Spence. "Assessment of the Contribution of Dispersion Interactions in the Energetics of Bergman Cyclization of Enediynes." (poster) 27th California State University Biotechnology Symposium; Santa Clara, California; January 2015.

35. <u>B. E. Silva*</u>, B. F. Gherman, J. A. Miranda. "Computational Study of the Mechanism of Metal-Salen Mediated Electroreductive Cyclization Reactions." (poster) 248th American Chemical Society National Meeting; San Francisco, California; August 2014.

36. <u>P. J. Marzouk**</u>, B. F. Gherman, J. D. Spence. "Time-Dependent Density Functional Theory Study of the Bergman Photocyclization Reactivity of Enediynes." (poster) 248th American Chemical Society National Meeting; San Francisco, California; August 2014.

37. <u>B. E. Silva*</u>, B. F. Gherman, J. A. Miranda. "Computational Study of the Mechanism of Metal-Salen Mediated Electroreductive Cyclization Reactions." (poster) 26th Annual Undergraduate American Chemical Society Research Conference for Northern California; San Francisco, California; May 2014.

38. <u>A. B. Ung*</u>, B. F. Gherman, J. D. Spence. "Computational Study of the Cyclization Reactions of Phenyl-Substituted Enediynes with Benzannelated and Quinoxaline-based Supporting Groups." (poster) 26th Annual Undergraduate American Chemical Society Research Conference for Northern California; San Francisco, California; May 2014.

39. <u>C. Q. Li**</u>, B. F. Gherman, J. D. Spence. "Computational and Experimental Study of the Thermal Cyclization of Enediynones and Dieneynones." (poster) 26th California State University Biotechnology Symposium; Santa Clara, California; January 2014.

40. <u>P. J. Marzouk**</u>, B. F. Gherman, J. D. Spence. "Time-Dependent Density Functional Theory Study of the Bergman Photocyclization Reactivity of Enediynes." (poster) 26th California State University Biotechnology

Symposium; Santa Clara, California; January 2014.

41. C. Q. Li**, B. F. Gherman, J. D. Spence. "Computational and Experimental Study of the Thermal Cyclization of Enediynones and Dieneynones." (poster) 44th Western Regional Meeting of the American Chemical Society; Santa Clara, California; October 2013.

42. P. J. Marzouk**, B. F. Gherman, J. D. Spence. "Photoexcitation of Enediyne Compounds and Implications for Their Bergman Cyclization Reactivity." (poster) 44th Western Regional Meeting of the American Chemical Society; Santa Clara, California; October 2013.

43. K. Minnick*, B. F. Gherman. "Using Computational Chemistry to Design an Optimal Biomimetic Ligand for the Active Site of the Peptide Deformylase Enzyme." (poster) 44th Western Regional Meeting of the American Chemical Society; Santa Clara, California; October 2013.

44. K. Minnick*, B. F. Gherman. "Using Computational Chemistry to Design an Optimal Biomimetic Ligand for the Active Site of the Peptide Deformylase Enzyme." (poster) 25th Annual Undergraduate American Chemical Society Research Conference for Northern California; Santa Clara, California; May 2013.

45. K. Minnick*, R. P. Fernandez*, B. F. Gherman, J. D. Spence. "Computational Analysis of Cyclization Reactions of Monosubstituted Enediynes and Comparison to Disubstituted Enediynes." (poster) 25th California State University Biotechnology Symposium; Anaheim, California; January 2013.

46. J. S. Fell**, B. F. Gherman, J. A. Miranda. "Mechanism of Electron Transfer in Metal-Salen Mediated Electroreductive Cyclizations." (poster) 25th California State University Biotechnology Symposium; Anaheim, California; January 2013.

47. P. J. Marzouk**, B. F. Gherman, J. D. Spence. "Photoactivation of Enediyne Compounds and Implications for Their Bergman Cyclization Reactivity." (poster) 25th California State University Biotechnology Symposium; Anaheim, California; January 2013.

48. S. Krawczyk*, B. F. Gherman, E. C. Brown. "Computational Investigation of the Effects of Hydrogen Bonding on Reaction Thermodynamics in a Carbonic Anhydrase Biomimetic System." (poster) 24th Annual Undergraduate American Chemical Society Research Conference for Northern California; Oakland, California; May 2012.

49. S. J. Bertolani*, A. E. Zamora*, B. F. Gherman. "Computational Investigation of Stabilizing Hydrogen Bonds in the Peptide Deformylase Reaction Mechanism." (poster) 24th Annual Undergraduate American Chemical Society Research Conference for Northern California; Oakland, California; May 2012.

50. M. Safi*, R. Fernandez*, B. F. Gherman, J. D. Spence. "Electronic Effects on the Cyclization Reactions of Enediynes Explored Through Modifications to the Enediyne Supporting Group." (poster) 24th Annual Undergraduate American Chemical Society Research Conference for Northern California; Oakland, California; May 2012.

51. S. Krawczyk*, B. F. Gherman, E. C. Brown. "Computational Analysis of Carbonic Anhydrase Biomimetic Reactivity via Novel Metal-Hydrosulfide Complexes." (poster) 24th California State University Biotechnology Symposium; Santa Clara, California; January 2012.

52. S. J. Bertolani*, A. E. Zamora*, B. F. Gherman. "Computational Study of Hydrogen Bonding Residues and Thiolate Coordination in the Active Site of Eubacterial Peptide Deformylase." (poster) 24th California State University Biotechnology Symposium; Santa Clara, California; January 2012.

53. S. Krawczyk*, B. F. Gherman, E. C. Brown. "Computational Analysis of Carbonic Anhydrase Biomimetic Reactivity via Novel Metal-Hydrosulfide Complexes." (poster) 43rd Western Regional Meeting of the American Chemical Society; Pasadena, California; November 2011. **undergraduate poster presentation award.

54. S. J. Bertolani*, A. E. Zamora*, B. F. Gherman. "Computational Study of Hydrogen Bonding Residues and Thiolate Coordination in the Active Site of Eubacterial Peptide Deformylase." (poster) 43rd Western Regional Meeting of the American Chemical Society; Pasadena, California; November 2011. **undergraduate poster presentation award.

55. J. S. Fell**, D. M. Steele*, B. F. Gherman. "Electronic Effects on the Reaction Mechanism of the Metalloenzyme Peptide Deformylase." (poster) 43rd Western Regional Meeting of the American Chemical Society; Pasadena, California; November 2011.

56. S. Krawczyk*, B. F. Gherman, E. C. Brown. "Computational Analysis of Metal-Hydrosulfide Complexes Supported by a Novel Carbonic Anhydrase Biomimetic Ligand System." (poster) 23rd Annual Undergraduate American Chemical Society Research Conference for Northern California; San Jose, California; May 2011. **awarded 1st place poster presentation.

57. R. Fernandez*, N. Korovina*, B. F. Gherman, J. D. Spence. "Computational Study of the Cyclization Reactions of Quinoxaline-Based Enediynes." (poster) 23rd Annual Undergraduate American Chemical Society Research Conference for Northern California; San Jose, California; May 2011.

58. V. A. Mendiola*, B. F. Gherman, J. A. Miranda. "Metal-Salens as Catalysts for the Reduction of Alkyl Halides: Analysis of Factors Affecting Reaction Pathway and Thermodynamics." (poster) 23rd California State

University Biotechnology Symposium; Anaheim, California; January 2011.

59. J. S. Fell**, D. M. Steele*, B. F. Gherman. "Electronic Effects on the Reaction Mechanism of the Metalloenzyme Peptide Deformylase." (poster) 23rd California State University Biotechnology Symposium; Anaheim, California; January 2011.

60. B. F. Gherman. "Computational Study of the Cyclization Reactions of Naphthyl-Substituted Enediynes." San Jose State University; San Jose, California; November 2010.

61. N. Korovina*, B. F. Gherman, J. D. Spence. "Computational Study of the Cyclization Reactions of Naphthyl-Substituted Enediynes." 22nd Annual Undergraduate American Chemical Society Research Conference for Northern California; Sacramento, California; May 2010.

62. V. A. Mendiola*, K. A. Pineda*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metals-Salens and Application to the Reduction of Alkyl Halides." 22nd Annual Undergraduate American Chemical Society Research Conference for Northern California; Sacramento, California; May 2010.

63. D. Steele*, B. F. Gherman. "DFT Computational Study of Biomimetic Model for the Metalloenzyme Peptide Deformylase." (poster) 22nd Annual Undergraduate American Chemical Society Research Conference for Northern California; Sacramento, California; May 2010.

64. N. Korovina*, B. F. Gherman, J. D. Spence. "Computational Study of the Cyclization Reactions of Naphthyl-Substituted Enediynes." (poster) 239th American Chemical Society National Meeting; San Francisco, California; March 2010.

65. V. A. Mendiola*, K. A. Pineda*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metals-Salens and Application to the Reduction of Alkyl Halides." (poster) 239th American Chemical Society National Meeting; San Francisco, California; March 2010.

66. N. Korovina*, B. F. Gherman, J. D. Spence. "Computational Study of the Cyclization Reactions of Naphthyl-Substituted Enediynes." (poster) 22nd California State University Biotechnology Symposium; Santa Clara, California; January 2010.

67. V. A. Mendiola*, K. A. Pineda*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metals-Salens and Application to the Reduction of Alkyl Halides." (poster) 22nd California State University Biotechnology Symposium; Santa Clara, California; January 2010.

68. N. Korovina*, B. F. Gherman, J. D. Spence. "Synthesis and photoreactivity of 1,2-bis(naphthalene-1-ylethynyl)benzene: A combined experimental and computational investigation." (poster) 238th American Chemical Society National Meeting; Washington, DC; August 2009.

69. A. E. Zamora*, B. F. Gherman. "Computational Study of the Effects of the Hydrogen Bonding Protein Environment on the Enzymatic Mechanism of Eubacterial Peptide Deformylase." (poster) 238th American Chemical Society National Meeting; Washington, DC; August 2009.

70. B. F. Gherman. "Using Computational Chemistry and Biomimetic Models to Investigate Catalysis and Enzyme Active Sites" Symposium on Learning and Industry Targeting Computational Chemistry Opportunities (Sylicco.09); University of California, Davis; Davis, California; July 2009.

71. N. Korovina*, B. F. Gherman, J. D. Spence. "Synthesis and photoreactivity of 1,2-bis(naphthalene-1-ylethynyl)benzene: A combined experimental and computational investigation." (poster) Symposium on Learning and Industry Targeting Computational Chemistry Opportunities (Sylicco.09); University of California, Davis; Davis, California; July 2009.

72. A. E. Zamora*, B. F. Gherman. "Computational Study of the Effects of the Hydrogen Bonding Protein Environment on the Enzymatic Mechanism of Eubacterial Peptide Deformylase." (poster) Symposium on Learning and Industry Targeting Computational Chemistry Opportunities (Sylicco.09); University of California, Davis; Davis, California; July 2009.

73. V. A. Mendiola*, K. England*, H. Kaur*, S. B. Bateni*, A. R. Mitchell*, A. T. Galatti*, M. H. Vu*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metal-Salens: A Dual Experimental / Computational Approach." (poster) Symposium on Learning and Industry Targeting Computational Chemistry Opportunities (Sylicco.09); University of California, Davis; Davis, California; July 2009.

74. N. Korovina*, B. F. Gherman, J. D. Spence. "Synthesis and photoreactivity of 1,2-bis(naphthalene-1-ylethynyl)benzene: A combined experimental and computational investigation." (poster) 21st Annual Undergraduate American Chemical Society Research Conference for Northern California; Moraga, California; May 2009.

75. A. E. Zamora*, B. F. Gherman. "Computational Study of the Effects of the Hydrogen Bonding Protein Environment on the Enzymatic Mechanism of Eubacterial Peptide Deformylase." (poster) 21st Annual Undergraduate American Chemical Society Research Conference for Northern California; Moraga, California; May 2009.

76. V. A. Mendiola*, K. England*, H. Kaur*, S. B. Bateni*, A. R. Mitchell*, A. T. Galatti*, M. H. Vu*, B. F.

Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metal-Salens: A Dual Experimental / Computational Approach." (poster) 21st Annual Undergraduate American Chemical Society Research Conference for Northern California; Moraga, California; May 2009.

77. T. C. Hatcher III*, A. E. Zamora*, B. F. Gherman. "Computational Study of the Enzymatic Mechanism of Eubacterial Peptide Deformylase via Functionalization of a Biomimetic Ligand." (poster) 21st California State University Biotechnology Symposium; Los Angeles, California; January 2009.

78. T. C. Hatcher III*, A. E. Zamora*, B. F. Gherman. "Computational Study of the Enzymatic Mechanism of Eubacterial Peptide Deformylase via Functionalization of a Biomimetic Ligand." (poster) 42nd Western Regional Meeting of the American Chemical Society; Las Vegas, Nevada; September 2008.

79. K. England*, H. Kaur*, A. R. Mitchell*, A. T. Galatti*, M. H. Vu*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metal-Salens: A Dual Experimental/Computational Approach." (poster) 42nd Western Regional Meeting of the American Chemical Society; Las Vegas, Nevada; September 2008.

80. M. F. Brown*, T. C. Hatcher III*, B. F. Gherman. "DFT Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase: Is the Identity of the Metal Center Significant?" 236th American Chemical Society National Meeting; Philadelphia, Pennsylvania; August 2008.

81. T. C. Hatcher III*, B. F. Gherman. "Computational Study of the Enzymatic Mechanism of Eubacterial Peptide Deformylase via Functionalization of a Biomimetic Ligand." (poster) 20th Annual Undergraduate American Chemical Society Research Conference for Northern California; Santa Clara, California; May 2008.

82. K. England*, H. Kaur*, A. R. Mitchell*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metal-Salens: A Dual Experimental/Computational Approach." (poster) 20th Annual Undergraduate American Chemical Society Research Conference for Northern California; Santa Clara, California; May 2008.

83. B. F. Gherman. "DFT Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase: Is the Identity of the Metal Center Significant?" Shasta College; Redding, CA; April 2008.

84. B. F. Gherman. "DFT Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase: Is the Identity of the Metal Center Significant?" 48th Sanibel Symposium; St. Simons Island, GA; February 2008.

85. M. F. Brown*, B. F. Gherman. "DFT Computational Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase." (poster) 20th California State University Biotechnology Symposium; Oakland, California; January 2008.

86. K. England*, H. Kaur*, A. R. Mitchell*, B. F. Gherman, J. A. Miranda. "Prediction of Reduction Potentials from Electron Affinities for Metal-Salens: A Dual Experimental/Computational Approach." (poster) 20th California State University Biotechnology Symposium; Oakland, California; January 2008.

87. B. F. Gherman. "DFT Computational Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase." California State University, Chico; Chico, CA; October 2007.

88. M. F. Brown*, B. F. Gherman. "DFT Computational Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase." (poster) Symposium on Learning and Industry Targeting Computational Chemistry Opportunities (Sylicco.07); University of California, Davis; Davis, California; July 2007. **awarded best ab initio molecular modeling poster.

89. M. F. Brown*, B. F. Gherman. "DFT Computational Study of a Biomimetic Model for the Metalloenzyme Peptide Deformylase." (poster) Nineteenth Annual Undergraduate American Chemical Society Research Conference for Northern California; Rohnert Park, California; May 2007.

90. B. F. Gherman, W. B. Tolman, and C. J. Cramer. "Evolution of Biomimetic Ligands for Modeling Dioxygen Activation at Monocopper Enzyme Sites." (poster) Twelfth International Congress of Quantum Chemistry; Kyoto, Japan; May 2006.

91. B. F. Gherman, W. B. Tolman, and C. J. Cramer. "Computational Modeling of Catalysis in Monocopper Enzymes: Dopamine β-Monooxygenase and Peptidylglycine α-Hydroxylating Monooxygenase." *Metalloprotein Interest Group*; University of Minnesota; Minneapolis, Minnesota; March 2006.

92. B. F. Gherman, W. B. Tolman, and C. J. Cramer. "Modeling Dioxygen Activation and Substrate Hydroxylation at Monocopper Enzyme Sites." (poster) Special Workshop on Theoretical and Computational Bridges: from Molecular Quantum Behavior to Biological Simulation; Indianapolis, Indiana; October 2005.

93. B. F. Gherman, W. B. Tolman, and C. J. Cramer. "Modeling Dioxygen Activation and Substrate Hydroxylation at Monocopper Enzyme Sites." (poster) Twelfth International Conference on Biological Inorganic Chemistry; Ann Arbor, Michigan; August 2005.

94. B. F. Gherman, W. B. Tolman, and C. J. Cramer. "Modeling Dioxygen Activation and Substrate Hydroxylation at Monocopper Enzyme Sites." (poster) Fifth Congress of the International Society for Theoretical Chemical Physics; New Orleans, Louisiana; July 2005.

95. B. F. Gherman, W. B. Tolman, and C. J. Cramer. "Modeling Dioxygen Activation by Biomimetic Cu(I) Complexes using DFT and CASPT2 Methods." University of Minnesota Waves & Beams seminar;

Minneapolis, Minnesota; March 2005.

96. <u>B. F. Gherman</u>, W. B. Tolman, and C. J. Cramer. "Modeling Dioxygen Activation at Monocopper Enzyme Sites." (poster) Computational Chemical Dynamics symposium; University of Minnesota and Minnesota Supercomputer Institute; Minneapolis, Minnesota; October 2004.

97. <u>B. F. Gherman</u>, W. B. Tolman, and C. J. Cramer. "Modeling Dioxygen Activation at Monocopper Enzyme Sites." (poster) International Society of Quantum Biology and Pharmocology (ISQBP) President's Meeting; Como, Italy; June 2004.

98. <u>B. F. Gherman</u>, W. B. Tolman, and C. J. Cramer. "Modeling 1:1 Adducts of O_2 with Cu." Indiana University inorganic seminar; Bloomington, Indiana; March 2004.

99. <u>B. F. Gherman</u>, S. J. Lippard, and R. A Friesner. "Substrate Hydroxylation in Methane Monooxygenase: Modeling via Quantum and Mixed Quantum/Molecular Mechanics Techniques." *Metalloprotein Interest Group*; University of Minnesota; Minneapolis, Minnesota; January 2004.

100. <u>B. F. Gherman</u>, S. J. Lippard, and R. A Friesner. "The Methane Monooxygenase Catalytic Cycle: Dioxygen Activation and Methane Hydroxylation." (poster) *Graduate Students in Chemistry in the Greater New York Metropolitan Area Poster Session*; New York, New York; February 2003.

101. <u>B. F. Gherman</u> and R. A. Friesner. "The Methane Monooxygenase Catalytic Cycle: Dioxygen Activation." *2002 Columbia University Biophysics Retreat*; New York, New York; September 2002.

102. <u>B. F. Gherman</u> and R. A. Friesner. "A Theoretical Study of the Methane Monooxygenase (MMO) Catalytic Cycle." (poster) *2001 Columbia University Biophysics Retreat*; New York, New York; June 2001.

AFFILIATIONS

1. Member of American Chemical Society since 1999.
2. Member of Council on Undergraduate Research since 2002.
3. Member of International Society of Quantum Biology and Pharmocology, 2004-2006.
4. Member of Society of Biological Inorganic Chemistry, 2005-2011.